Prediction of Multifunctional Mo_4SiC Monolayer Material with Intrinsic Superconductivity, Giant Negative Poisson's Ratio, and Promising Hydrogen Evolution Reaction Performance

Fig.S1. Electronic band structures of the Mo_4SiC monolayer calculated using different methods: PBE (black), HSE06 (red), and DFT+U with U = 2, 4, and 6 eV (blue, green, and orange lines, respectively). The Fermi level is set to 0 eV. All methods consistently predict a metallic character for the material, as bands cross the Fermi level.

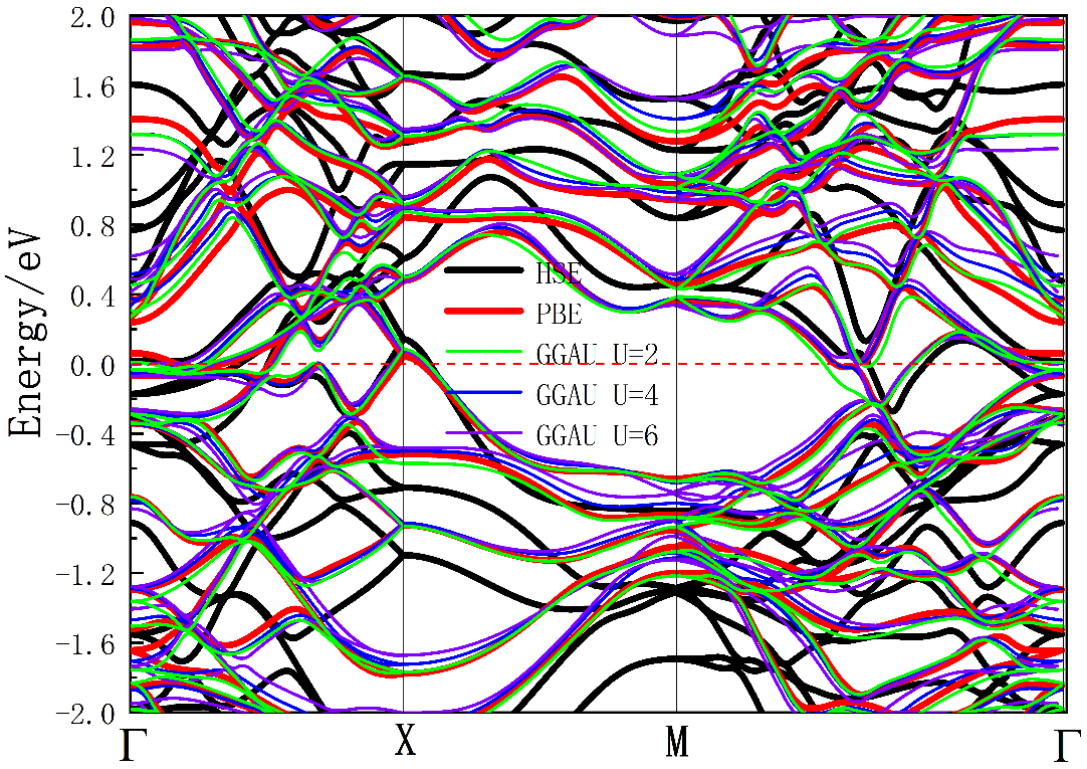

Fig.S2. Low-energy structures of Mo_4SiC identified through the CALYPSO structural search, viewed along different orientations: top view and side views of distinct configurations. The relative energies (in meV/atom) with respect to the ground state are indicated below each structure, highlighting the identified most stable configuration.

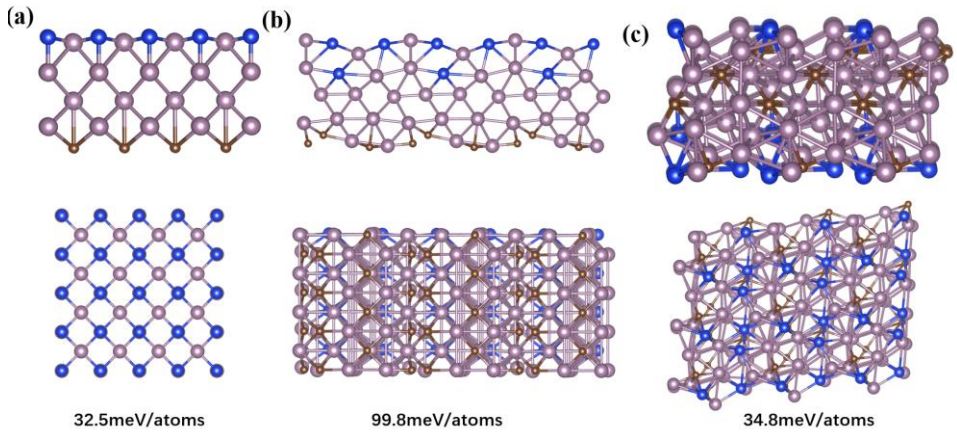

Fig.S3 Structural stability of the Mo_4SiC monolayer during *ab initio* molecular dynamics (AIMD) simulations with H or H_2O adsorption. (a, b) Representative atomic structure snapshots (top) and the corresponding temperature fluctuations (bottom) from the 300 K AIMD simulations for the cases of (a) H and (b) H_2O adsorption on the Mo_4SiC surface. The atomic configurations (Snapshots) demonstrate that the monolayer framework remains intact without reconstruction or degradation throughout the 2 ps simulation. The temperature profiles confirm the system's dynamical behavior under the NVT ensemble. Color code for atoms: Mo (brown), Si (blue), C (pink), H (white), O (red).